Department Of Energy

Computational Science Graduate Fellowship

Guide for Practicum Advisor

September 21, 2008

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Executive Summary

The DOE Computational Science Graduate Fellowship (DOE CSGF) program began in 1991. Since then over 200 exceptionally talented students have participated and graduates are now performing valuable work at DOE laboratories, universities, and industry. This is a very selective program; last year only ~5% of the applications were successful. Each student agrees to perform a research practicum at a participating DOE laboratory.

This guide suggests "good practices" to increase the likelihood that the practicum is rewarding for all involved. It includes a summary of the practicum advisor's responsibilities, a discussion of resources available to help the practicum advisor be successful, and concludes with a collection of observations from past practicum advisors.

Introduction

Each DOE CSGF student represents a significant investment by DOE. The fellowship provides full tuition and fees for the fellow at the school of their choosing for four years. In addition to tuition support fellows receive an annual stipend that is set to be among the most generous offered for graduate work (for the FY2008 – 2009 year, it will be $32,400), a small sum to support professional expenses, and up to $2475 towards the purchase of a workstation. This investment is designed to encourage the best university students to continue on to advanced studies in the computational sciences. During the research practicum, the fellowship provides each student with a stipend increment to cover the additional costs associated with living away from their university.

When a student accepts a DOE CSGF award she also agrees to accept guidance from a select group of computational scientists (the DOE CSGF Steering Committee) and complete a Program of Study that the Steering Committee approves. DOE's interest in supporting these students is not purely altruistic. DOE also uses this program to introduce students to the DOE laboratories and each fellow is required to perform a research practicum at one of these laboratories. The practicum, while fulfilling the purpose of familiarizing fellows with the DOE laboratory system, is also meant to expand the fellow's professional horizons. All proposed practicum research will be reviewed to ensure that it isn't a simple extension of the student's thesis work.

Responsibilities of the practicum advisor

In summary, your responsibilities as practicum advisor are:

i. To accurately communicate your group's activities to your site's Practicum Coordinator.
ii. To craft a research experience that is both useful for the fellow and supports your group's mission.
iii. To accurately convey the special nature of DOE laboratory research.
iv. To evaluate the student's practicum research and convey your impressions to the Practicum Coordinator and the DOE CSGF Program Coordinator.

Resources

DOE CSGF Practicum Coordinator

Each participating DOE Laboratory has named a DOE CSGF Practicum Coordinator who is an interface between the laboratory, the fellows, and the program administrative staff. The Practicum Coordinator is also a resource for both you and the fellows at your laboratory. You should help the Practicum Coordinator accurately represent your group's research to prospective students so that they can choose their assignments wisely. It's also important to keep the Practicum Coordinator aware of the fellow's achievements so that program results can be briefed to laboratory management and other scientists at the laboratory.

University Thesis Advisor

Each fellow is a full-time graduate student and has a thesis advisor. While practicum research should not be directly related to the fellow's thesis topic, the thesis advisor should be very interested in what the fellow does at your site and can help craft a productive experience for all involved.

DOE CSGF Resources

The Krell Institute, who administers the DOE CSGF program for DOE, employs a Program Coordinator, Jeana Gingery, whose full-time job is to help insure that everything goes smoothly in the program. If you or your student needs help and/or advice at any time you are invited to contact her (515-956-3696, or gingery@krellinst.org). Ms. Gingery has prepared information about the housing resources available at each participating site and you should make your fellow aware of this information.

Things to do before the practicum

Your participation in the DOE CSGF practicum offers many opportunities. One is to establish or strengthen relations with computational science leaders in academia. Arrange to meet, via telephone or in person, with both the fellow and the fellow's university advisor as soon as possible to plan a meaningful practicum. Once a topic of study has been identified, review the fellow's academic background and approved Program of Study (POS) and suggest additional course work or reading to help the fellow prepare to participate in your group's work.

The DOE CSGF program provides funding for fellows to visit sites before the practicum begins to help plan for the practicum. *Please alert the fellow to this opportunity.*

You or your designee should meet with your Practicum Coordinator before the fellow arrives to make sure that administrative details (site access, computer accounts, necessary briefings, work space access, etc.) are addressed so that fellows can get to work when they arrive. This will not be a surprise since the Practicum Coordinator has previously signed documentation with this information, but it will help insure that everything is ready.

Your site's Practicum Coordinator will alert laboratory administrative staff that the fellow will be working with you and when the fellow is expected to arrive. Hopefully this will allow some of the logistical requirements your site has established to be completed before the fellow arrives. **You will need to establish a physical workplace for your fellow and arrange for computer access, networking, etc**. **It is best to make these arrangements before the fellow arrives.** It is also useful to notify others in your group about the fellow and discuss your expectations for the fellow with them.

If the practicum occurs during a period when you will be absent (vacation, extended work-related travel) or heavily engaged in other work, you should arrange for someone in your group to supervise the fellow and convey that information to everyone concerned.

If possible, start informing the fellow about group and relevant laboratory activities prior to the fellow's arrival at your lab. Anything that familiarizes the fellow with your local environment will help make the transition to your worksite more effective. If group or laboratory meetings are advertised via e-mail, consider putting the fellow on the distribution list prior to the practicum so that the fellow gets in the spirit of things before actually arriving on site. (You might consider a reciprocal arrangement so that you are informed about the seminars at the fellow's university.)

If your group imposes restrictions on access to or dissemination of information you will need to explicitly discuss these policies with the fellow. Make certain that the Practicum Coordinator and the fellow know and understand the special responsibilities associated with

work in your group. Responsible computer use, computer security, and special group practices should be explicitly discussed and understood by all.

With regard to intellectual property, the fellow's Terms of Appointment state:

In recognition of the statutory intent set forth in Title 35 United States Code Section 212, the fellow acknowledges that this appointment is considered to be in the nature of a scholarship, fellowship, training grant, or other funding agreement made on behalf of a Federal agency primarily to an awardee for educational purposes, and therefore, no provision shall be contained herein, nor shall any section be construed as permitting or authorizing, the Federal agency to assert any rights to inventions made by the awardee.

The fellows are advised that their university or practicum site may have special rules in force to govern the use of information and that there are potentially severe penalties for violating those rules, particularly for classified information.

Expectations

It's important to develop reasonable expectations of what a DOE CSGF fellow can accomplish during the practicum and to communicate that to members of your research team. Previous fellows have been able to publish research from their summer experience, develop code modules that advanced the team's simulation capabilities, and introduced the team to algorithms and other software that proved beneficial to the team. When other fellows were less successful, it could usually be traced to insufficient logistical planning prior to the fellow's arrival or to some confusion between the fellow and her advisor and the practicum advisor.

The DOE CSGF program *will support a fellow at a site for longer than 12-weeks and encourages that fellows consider participating in a second practicum.* If the fellow begins to develop exciting results towards the end of the practicum it is possible, with the concurrence of the thesis advisor to extend the practicum and the DOE CSGF program can provide additional funds to support the fellow's extra living expenses.

Also note that it is good pedagogic practice to arrange the student's work so that a discrete part of a project can be completed within the practicum period.

What to do during the practicum.

Make certain that the fellow knows and understands the special responsibilities associated with work in your group. Even though computer security and responsible computer use policies may be part of general laboratory training, it is important that these issues be discussed within the context of your group's practices. Many students will be familiar with a much more open computing environment than exists at your site and you should be absolutely certain that they understand the restrictions on computer use in your lab.

The fellow should participate in your group's regular meetings, can be encouraged to present a talk on their thesis work, and should keep up with the literature. Make information available about complementary research going on at nearby universities and laboratories to facilitate opportunities for the fellow to broaden the practicum experience.

What to do after the practicum.

It is important for you to provide an evaluation of the practicum experience to the fellow, to DOE CSGF program staff, and to your Practicum Coordinator. After the conclusion of the

practicum, the Program Coordinator will send you the address of a secure URL site where you will find an evaluation form for the practicum. Please fill it out.

Many Practicum Advisors have continued their relationship with fellows after the practicum. Where applicable, consider continuing collaboration by:

i.   Encouraging the fellow to consider a 2nd practicum in the group.
ii.   Collaborating on preparation of papers, conference presentations, etc.
iii.   Developing good rapport with the fellow's faculty advisor. For example, plan a visit to the university and present a talk on current research.
iv.   Providing funds for follow-up visits to the lab to continue work.
v.   Arranging a post-doctoral position for the fellow following graduation.
vi.   Continue interactions with faculty advisor through collaborative grants, etc.

Predictions
No one can predict what your experience with a fellow will be like. However, what you do can have a significant impact on the practicum experience for you, your organization and the fellow. Many Practicum Advisors have had very positive experiences with their fellows including joint publications and extended collaborations and some have made very little of the opportunity before them. We hope that you take advantage of this opportunity and gain benefits for yourself, your lab, the DOE and the fellow.

Our database of practicum advisor comments for current fellows extends to over 43 pages. Answers to the question, "Did the fellow contribute to your programs? Characterize the fellow's performance." may help you estimate what your experience will be like. Responses to the question are provided in the following Appendix [A] (with suitable scrubbing to protect the innocent).

APPENDIX A

Answers to the question: "Did the fellow contribute to your programs? Characterize the fellow's performance."

1. The fellow performed excellently. He was everything an advisor could want; hard working, motivated (worked on weekends), creative, responsible, and intelligent. His contributions were extremely important to our project (and I'm sad to see him go!).

2. The student's project was selected to fit into his current research activities and his work could be useful in several of our division's ongoing programs in computational materials science. The fellow is an extremely bright, hardworking student and his performance at our facility was good.

3. The fellow indirectly contributed in a very positive way to our developing program for radiation transport methods for medical applications. His performance was very good. He is diligent, industrious, shows initiative, works well independently, and works well with others. He is both mature and dependable.

4. Yes. I rate his performance level as very high. He had lots of ideas and was a significant contributor

5. The fellow brought expertise in the area of combustion to our program. Her performance was commendable.

6. The fellow's work did not contribute directly to our programs here at LLNL since the sort of computational biology problem that he is addressing is not in the scope of work at the Laboratory. However, the fellow's work is of interest to the SAMRAI team in that it stresses our software in new ways by applying it to new problems. He is a bright, young computational mathematician and a very hard worker. He learned a lot of new things while at LLNL and performed excellently.

7. Excellent.

8. The fellow is an extremely bright individual with excellent computational science and applied mathematics skills. I was truly impressed with the speed with which he became familiar with the SAMRAI library and developed a working code. I genuinely look forward to having a longer-term interaction with the fellow as we will continue to work together on the AMR implementation of his electrophysiological heart model.

9. Yes, he brought C++ programming experience as well as applications expertise to the project. His performance was outstanding.

10. Yes. He worked with very little direct supervision. He's very motivated. His performance was outstanding.

11. The fellow worked enthusiastically and competently on this modeling, which is a very hard problem for the highly non-equilibrium plasmas of importance to several laser-target physics projects here. His work was excellent.

12. We are strongly interested in the availability of such improved Quantum Monte Carlo techniques in our program, and thus any developments in this area are important. The fellow's performance was excellent.

13. Yes. Very satisfactory.

14. Yes. The fellow is a self starter, quick to tackle problems, has excellent facility with computational tools, and a great attitude towards his work. He will be a first rate computational scientist.

15. Yes. The fellow follows directions and interacts with others well.

16. The highest performance. I have been a professor in the past, and the fellow was the brightest student I have ever worked with. He came up to speed quickly and surpassed me.

17. The linkage analysis code development project was a new effort for Sandia, starting this summer at the same time the fellow visited. Considerable progress was made and the fellow was the key developer and scientific lead on the project. His enthusiasm and biology knowledge were key to getting this effort off the ground.

18. The fellow has provided valuable contributions to our work, both in the form of software development for multidimensional applications and relating the work to existing techniques for reactive transport problems. His performance has been outstanding. He is innovative and a self starter.

19. The fellow took a difficult, ill-formed problem and made real contributions. He developed a novel approach to computing a global dexterity index with obstacles. He worked well with other researchers here at Sandia and produced interesting results.

20. The work that was performed was in support of 3 Sandia LDRD (Laboratory Driven Research and Development) projects. The fellow's performance was on par with that of members of the technical staff of Sandia. The fellow is very hard working, and a promising student. His deep understanding of Fluid Mechanics and innovative thinking ranks him among the very best students employed at Sandia.

21. Both his development work and issues he identified and resolved during the project provided useful contributions to capabilities I will need in the future. The fellow is hard-working, insightful, and productive.

22. Our organization has a strong interest in cohesive approaches to modeling fracture. Since the approach is physics-based rather than being phenomenological, we have an especially strong interest in validation of the models against experimental observations. The fellow's work in both the experimental and numerical aspects of the mica peel problem gave her a unique perspective on the behavior she observed. She displayed a high degree of self-initiative and communicated effectively with me and other members of the Sandia staff.

23. The fellow's energy, enthusiasm, creativity, and insights were exceptional. He quickly educated himself on a challenging topic, worked hard and effectively to solve many problems that arose during the effort, and contributed valuable ideas that will have lasting impact on future work in this area. The results he obtained provide a sound starting point for a newly initiated internal Sandia project that will further develop the modeling approach.

24. The fellow made strong contributions to our program. I would characterize his performance as excellent.

25. The fellow's concentrated effort during the summer brought this particular project to a feasibility decision point; which is very valuable to my program. The fellow was extremely hard working, independent, responsible and creative.

26. The fellow did compile a database of RNA genes and non-coding sequences in yeast (an important and difficult step). She also developed software to extract input parameters in an automatic way and made initial steps in machine learning of RNA genes. The fellow did most of the work in the last couple of weeks of the practicum. Earlier, the fellow was distracted by the new environment, personal obligations, and graduate student obligations with her advisor and collaborators. Overall, the fellow made some contribution to the program but did not have sufficient time to complete the project.

27. He was a very successful student.

28. The fellow performed well. She very quickly learned to use the first-principles code and started performing calculations of the Quantum Well States. She was very organized in her work and very productive, performing a large number of simulations of different systems during her short visit. We have a program to perform theoretical calculations related to experiments at the ALS to which she greatly contributed. She also interacted well with other postdocs working with us.

29. The fellow is a bright person, and contributed reasonably well to my program. However, I thought that she had a fairly large amount of travel and other commitments (on top of my own summer travel) that did not make for the best conditions for advancing our original goals.

30. Yes, the fellow contributed to our program. She developed a new algorithm and implemented it within our code framework, enabling us to share her advances and to use the new methodology when our research needs require it.

31. Yes, the fellow contributed to our developing understanding of quasi-chemical theories based on molecular physics at molecular resolution. She worked out a series of background statistical mechanics problems of increasing difficulty. She tackled these problems with energy and skill. Her efforts suggested to us a 'self-consistent cavity field' approach currently under development that clearly will revolutionize basic problems of theory of liquids, in particular the description of the paradigmatic hard sphere fluid.

32. We are interested in such discretizations for application to radiation transport calculations on AMR meshes. The fellow did a great deal of analysis and obtained some very useful theoretical results. He worked independently and required minimal supervision. I was extremely pleased with his performance. He is one of the best graduate students I have ever worked with.

33. As a result of the fellow's programming skills we were able to make substantial progress in parallelizing the computer code FLOTRAN. This code is used in a number of DOE funded projects. His performance was engaging, highly motivated, and required substantial effort on my part to stay one step ahead---which was not always possible.

34. The fellow had a very good visit to Los Alamos both in terms of her productivity and her learning experiences. She learned very readily how to use in an effective way the Gaussian98 software, other related programs to prepare and interpret calculations, and the workstation environment in the group (which changed from a SGI cluster to a Linux cluster over the course of her stay!). Her work contributed to ongoing efforts at the Laboratory (a) in helping experimentalists performing spectroscopic studies on these molecules at Los Alamos to interpret their results and (b) in helping gauge how theoretical methods could be applied to such complexes which are of possible interest in new energy technologies such as light emitting diodes. Overall I think her performance was especially noteworthy in terms of her dedication and resolve, since during the latter part of her practicum she was balancing her normal activities with responsibilities involving family medical issues.

35. Yes. The fellow met expectations.

36. Yes. The fellow established a much needed connection between the applied mathematics/ mechanical engineering way of modeling phase transformations with that of the way of physicists, i.e. a strain order parameter based Ginzburg-Landau model. It directly contributed to our program on modeling phase transformations. His performance was excellent.

37. The fellow's work is being submitted for publication in Physical Review D as first author. From the very first day at work, the fellow jumped into this project with both feet! I have only seen one other student perform at such a level in the 12 years I have mentored students at the Laboratory. He became the primary code developer on a team of three Technical Staff Members. The project, which started anew just a month or so before his practicum started, has been launched into one of the three major thrusts of my group. The fellow had much to do with its initial success. He is a highly qualified numerical relativist. I was mostly impressed with the quickness he was able to master a

field that was completely foreign to him (relativistic hydrodynamics). His dissertation deals with the collision of two black holes, thus no matter. The project he chose to work on during his practicum dealt exclusively with matter in a general relativistic gravitational field.

38. Absolutely. The fellow's performance was excellent. I would rate him as being as skilled and productive as some postdoctoral fellows in computational astrophysics.